A New Technique for Solving Poisson's Equation on Domains of Arbitrary Aspect Ratio

Robert Ryne
Lawrence Berkeley National Laboratory

SciDAC Accelerator Modeling Project Seminar

June 5, 2003

Acknowledgements

- **Work performed in collaboration with**
  - J. Qiang, LBNL
  - R. Gluckstern, U. Maryland, retired

Modeling systems with large aspect ratios is a difficult and important issue

- Issue: Poisson solvers used in PIC codes often fail when grid aspect ratio >> 1
- Relevance: Many important problems involve extreme aspect ratios:
  - Long beams in rf circular accelerators: length ~1m; radius ~1mm
  - Flat beams (as at interaction point of lepton colliders)
  - Beams in induction linacs: length~ 10s of meters; radius ~ cm
  - Galaxies
- Standard grid-based approaches use very large # of grid points in the long dimension, leading to prohibitively long run times
- As a result, it is <u>extremely difficult or impossible</u> to model high aspect ratio systems accurately using standard grid-based approaches, even on terascale computers

A potential "brick wall" in the road to large-scale space-charge simulations of beams in circular machines

- mid-to-late1990s : parallel high current linac modeling codes
  - Example: IMPACT code
  - linac length ~km; ~1000s steps (Poisson solves); ellipsoidal bunches
- Early 2000s:
  - Parallel weak-strong and strong-strong beam-beam simulations in colliders
  - Major advances including first-ever million-particle, million-turn strong-strong beam-beam simulation (J. Qiang)
- 2000+ : advance to modeling beams with space charge in circular machines
  - Very long simulations: 1000's to millions of turns
  - More difficult Poisson problem if aspect ratio is large
  - Keeping grid near-square would involve ~10-1000x more grid points

- (>1000s more steps) x (10-1000x more grid points) □ *10^4 to >10^6 times more challenging than linac modeling*
- Will not get this advance from hardware alone; also need <u>advances in algorithms</u>

Poisson Problem: Observation

- **The Green function, G, and source density, ρ, may change over vastly different scales**
- **In simple geometries G is known apriori; ρ is not**

We should use our full knowledge of G, as needed, to obtain accurate, efficient, and robust solution of the Poisson problem

- **Example: 2D Poisson equation in free space**

$$\phi(x,y) = \int G(x - x', y - y')\rho(x', y')\,dx'\,dy'$$

$$G(x - x', y - y') = \frac{1}{2}\ln((x - x')^2 + (y - y')^2)$$

Standard Approach (Hockney and Eastwood)

$$\phi(x,y) = \int G(x - x', y - y')\rho(x', y')\,dx'\,dy'$$

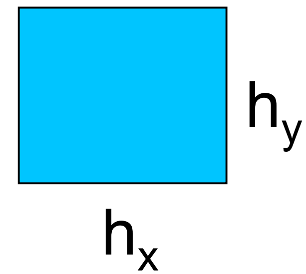
$$\Downarrow$$

$$\phi_{i,j} = \sum G_{i-i',\,j-j'}\,\rho_{i',\,j'} \qquad\qquad G_{0,0} = G_{0,1}$$

- **approach makes use of only partial knowledge of G**
- **equivalent to trapezoidal rule to approximate the convolution integral**
- **Cutoff at (x,y)=(0,0); isotropy issue for large aspect ratio**
- **error depends on how rapidly the integrand, ρG, varies over an elemental cell**
  - If ρ changes slowly we might try to use a large grid spacing; but this can introduce huge errors due to the change in G over a cell length

Cellular Analytic Convolution (CAC)

- Assume ρ varies in a prescribed way in each cell
- Use analytic Green function to perform the convolution integral exactly in each cell, then sum over cells
- Example: linear basis functions to approximate ρ.



$$\phi(x_i,y_j) = \frac{1}{h_x h_y}\sum_{i',j'} \rho_{i,j}\int_0^{h_x} dx'\int_0^{h_x} dy'(h_x - x')(h_y - y')G(x_i - x_{i'} - x', y_j - y_{j'} - y') +$$

$$\frac{1}{h_x h_y}\sum_{i',j'} \rho_{i+1,j}\int_0^{h_x} dx'\int_0^{h_x} dy'\, x'(h_y - y')G(x_i - x_{i'} - x', y_j - y_{j'} - y') +$$

$$\frac{1}{h_x h_y}\sum_{i',j'} \rho_{i,j+1}\int_0^{h_x} dx'\int_0^{h_x} dy'(h_x - x')y' G(x_i - x_{i'} - x', y_j - y_{j'} - y') +$$

$$\frac{1}{h_x h_y}\sum_{i',j'} \rho_{i+1,j+1}\int_0^{h_x} dx'\int_0^{h_x} dy'\, x' y' G(x_i - x_{i'} - x', y_j - y_{j'} - y')$$

- Shifting the indices results in a single convolution* involving an integrated effective Green function: $\phi_{i,j} = \sum_{i',j'} G^{eff}_{i-i',j-j'}\rho_{i',j'}$

* plus possible boundary corrections involving single (not double) sums

G^{eff} consists of 4 terms: what are they?

- **1st term: Indefinite integral is function of $(x_i - x_{i'}, y_j - y_{j'}) = (a,b)$ evaluated at** (a,b), $(a-h_x,b)$, $(a,b-h_y)$, $(a-h_x,b-h_y)$

$$
\begin{aligned}
&-\frac{x^3}{9} - \frac{1}{4}\,(\mathrm{hx} - a)\,x^2 + \\
&\frac{1}{12}\,(-3\,a + 3\,\mathrm{hx} + 2\,x)\,\log(x^2 + y^2)\,x^2 + \\
&\frac{1}{6}\,y\,(-3\,b + 3\,\mathrm{hy} + 2\,y)\,x - \\
&\frac{1}{2}\,(b - \mathrm{hy})\,(-2\,a + 2\,\mathrm{hx} + x)\,\tan^{-1}\left(\frac{y}{x}\right)x - \\
&\frac{1}{6}\,(2\,y^3 - 3\,b\,y^2 + 3\,\mathrm{hy}\,y^2)\,\tan^{-1}\left(\frac{x}{y}\right) - \\
&\frac{1}{4}\,(a\,y^2 - \mathrm{hx}\,y^2 - 2\,a\,b\,y + 2\,b\,\mathrm{hx}\,y + 2\,a\,\mathrm{hy}\,y - 2\,\mathrm{hx}\,\mathrm{hy}\,y) \\
&\log(x^2 + y^2)
\end{aligned}
$$

No interaction cutoff at short distances

- Formulas looks like they have singularities, but result must be finite
- In general, limiting form is needed in 4 cases:
  - $(x_i - x_{i'} \to 0,\ y_j - y_{j'} \to 0), (x_i - x_{i'} \to h_x,\ y_j - y_{j'} \to 0), (x_i - x_{i'} \to 0,\ y_j - y_{j'} \to h_y), (x_i - x_{i'} \to h_x,\ y_j - y_{j'} \to h_y)$
- Example: $(x_i - x_{i'} \to h_x,\ y_j - y_{j'} \to h_y)$

$$
\begin{aligned}
\frac{1}{6}\Bigg(&-16\,\mathrm{hy}^3\,\mathrm{ArcTan}\left[\frac{\mathrm{hx}}{2\,\mathrm{hy}}\right] + 12\,\mathrm{hy}^3\,\mathrm{ArcTan}\left[\frac{\mathrm{hx}}{\mathrm{hy}}\right] - \\
&2\,\mathrm{hy}^3\,\mathrm{ArcTan}\left[\frac{2\,\mathrm{hx}}{\mathrm{hy}}\right] - 24\,\mathrm{hx}^2\,\mathrm{hy}\,\mathrm{ArcTan}\left[\frac{\mathrm{hy}}{2\,\mathrm{hx}}\right] + \\
&36\,\mathrm{hx}^2\,\mathrm{hy}\,\mathrm{ArcTan}\left[\frac{\mathrm{hy}}{\mathrm{hx}}\right] - 12\,\mathrm{hx}^2\,\mathrm{hy}\,\mathrm{ArcTan}\left[\frac{2\,\mathrm{hy}}{\mathrm{hx}}\right] + \\
&\mathrm{hx}^3\,\mathrm{Log}[\mathrm{hx}^2] - 4\,\mathrm{hx}^3\,\mathrm{Log}[4\,\mathrm{hx}^2] - \\
&2\,\mathrm{hx}^3\,\mathrm{Log}[\mathrm{hx}^2+\mathrm{hy}^2] + 6\,\mathrm{hx}\,\mathrm{hy}^2\,\mathrm{Log}[\mathrm{hx}^2+\mathrm{hy}^2] + \\
&8\,\mathrm{hx}^3\,\mathrm{Log}[4\,\mathrm{hx}^2+\mathrm{hy}^2] - 6\,\mathrm{hx}\,\mathrm{hy}^2\,\mathrm{Log}[4\,\mathrm{hx}^2+\mathrm{hy}^2] + \\
&\mathrm{hx}^3\,\mathrm{Log}[\mathrm{hx}^2+4\,\mathrm{hy}^2] - 12\,\mathrm{hx}\,\mathrm{hy}^2\,\mathrm{Log}[\mathrm{hx}^2+4\,\mathrm{hy}^2] - \\
&4\,\mathrm{hx}^3\,\mathrm{Log}[4\,\mathrm{hx}^2+4\,\mathrm{hy}^2] + 12\,\mathrm{hx}\,\mathrm{hy}^2\,\mathrm{Log}[4\,\mathrm{hx}^2+4\,\mathrm{hy}^2]\Bigg)
\end{aligned}
$$

Cost and Accuracy; Improvement over Hockney Approach

- Cost: Computing the elemental integrals can be done via analytical formulae or by numerial quadrature
  - Requires more FLOPS than simply using G_{ij} but…
  - when the grid is fixed, needs to be done once at the start of a run. Amortized over many time steps, does not significantly impact run time.
  - Note well: sensitivity to roundoff for large aspect ratios. Care required!

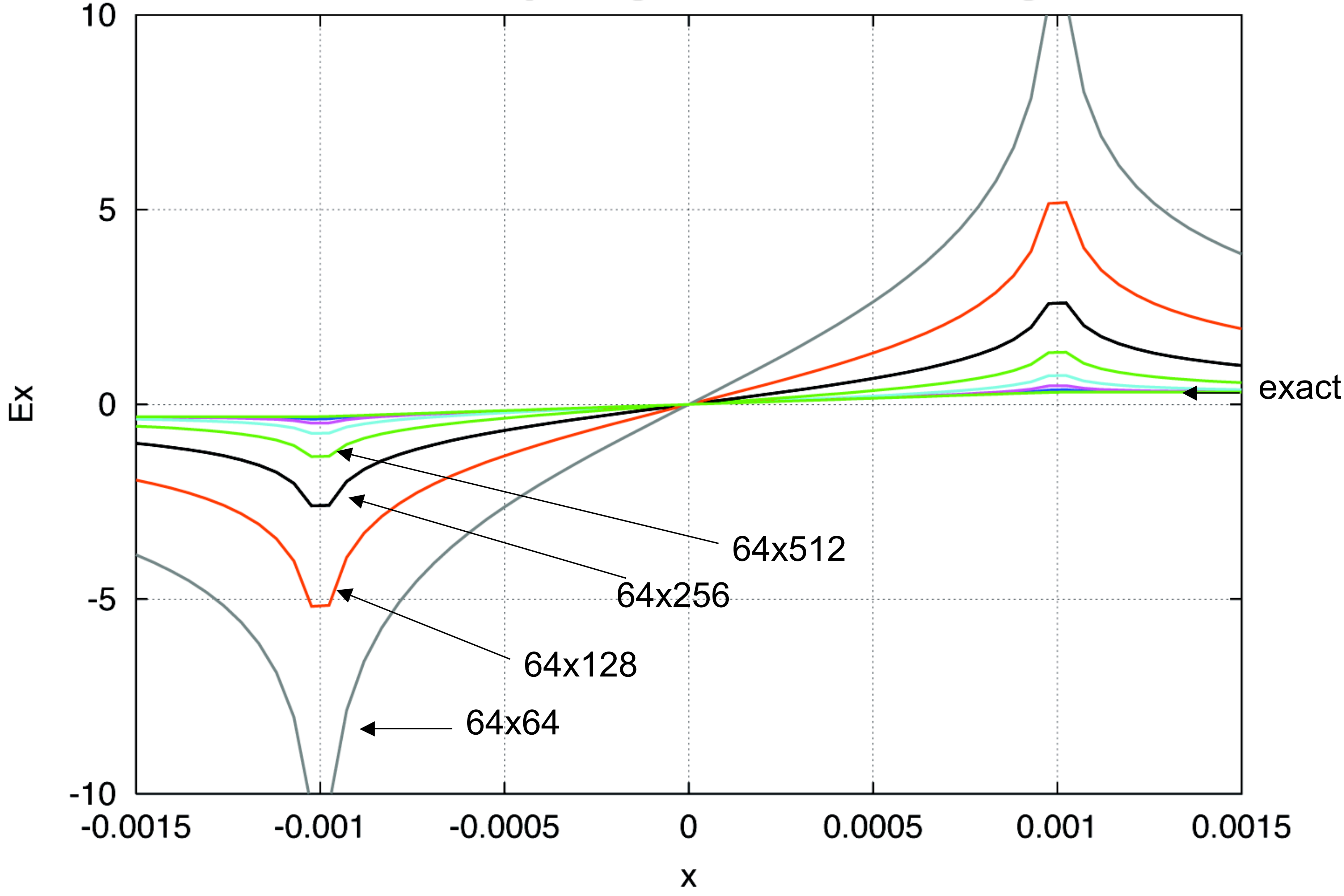
- Accuracy: Method works well as long as the elemental integrals are computed accurately and as long as the grid and # of macroparticles are sufficient to resolve variation in
  - maintains accuracy even for extreme aspect ratios (>1000:1)

As a result, new method performs orders of magnitude better than the standard convolution algorithm for realistic problems involving large aspect ratios

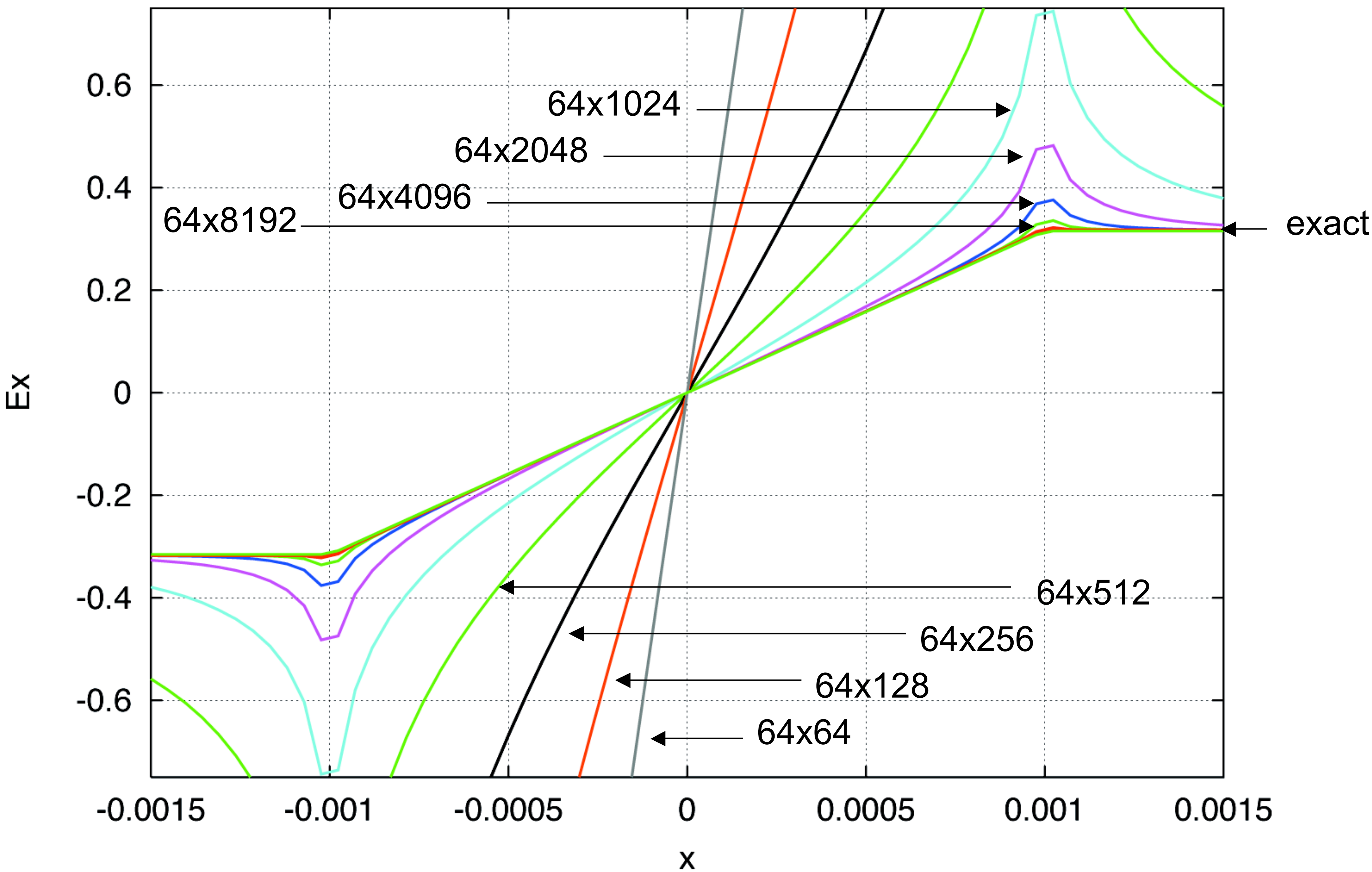
Example: Uniformly filled 2D ellipse

- **Aspect ratio is 1:1000**
  - x_{max}=0.001, y_{max}=1
- **Calculation of fields using (1) standard Hockney algorithm and (2) new approach**
  - In both cases, performed convolutions for the fields directly (rather than calculating the potential and using finite differences to obtain fields)
- **Calculation performed on a grid of size ±0.0015 x ± 1.5 using a mesh of size**
  - Hockney: 64x64, 64x128, 64x256,…, 64x16384
  - New approach: 64x64

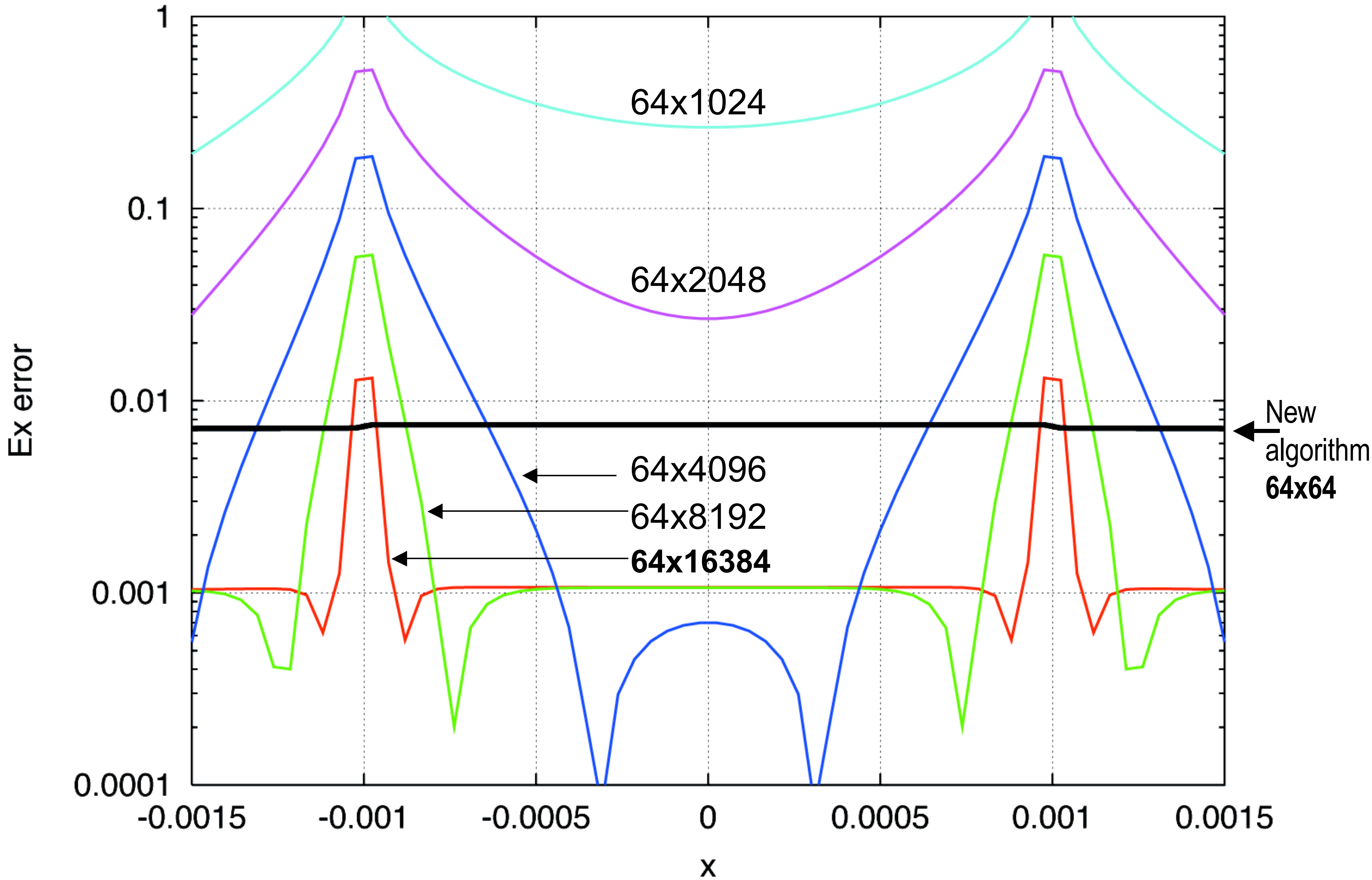
1:1000 test case; Ex vs. x: Standard Hockney Algorithm has huge errors



Ex vs. x : Reduced Vertical Scale



Old algorithm has large errors until grid size reaches ~ 64x8192.
New algorithm has excellent accuracy on a grid as small as 64x64



Comparisons with other methods

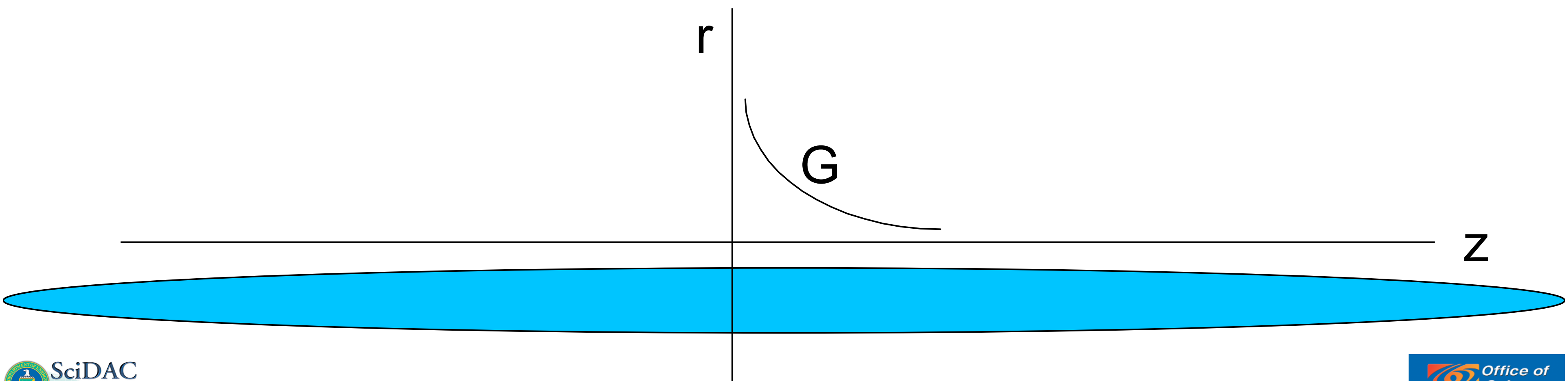
- **Comparison with the finite element method:**
  - New method uses basis functions, but there is no variational quantity to be numerically minimized and no linear system to be solved
    - This is done analytically
- **Comparison with the finite difference method:**
  - FD approximates: (1) continuous operators by stencils on grids, and (2) sources by values at grid points
    - Error in (1) depends on behavior of the solution, □, compared with the FD approximation to □^{2}
  - Error in new approach is *source-limited*, i.e. it only depends on the deviation of the source, □, from the assumed functional form
    - No issue with anisotropy except indirectly through the representation of □

Comment on Direct Convolution Methods

- Would not be generally useful except for the key fact that *a discrete convolution can be turned into a cyclic convolution through zero padding and periodization of G*
  - Turns N^2 method into N log N at the price of grid doubling*
  - Works when G=G(x-x')
  - Also works when G=G(x+x')

Future Directions

- **Extension to 3D straightforward but messy**
  - Formulas have been generated using a symbolic math program
  - Implementation underway
- **Question: Can this general approach (i.e. using full analytical knowledge of G) be used in other simple geometries?**
  - Can do Dirichlet in a box (write G as sum of convolutions/correlations)
  - Long beams in pipes:
    - Analytic approach to integratioin is crucial since **G** and may vary on vastly different scales
    - potential performance increase by making use of shielding (exponential falloff) in the long direction to discard terms beyond a certain distance from the source



Extension to Beams in Pipes

- CAC provides a crucial advantage, since the Green function falls off exponentially in z, though $\rho(z)$may change slowly over meters
- Due to shielding, sum can be truncated in the “long” direction:

$$\phi_{i,j} = \sum_{i'=1}^{N_x} \sum_{j'=j}^{j \pm j_{cutoff}} G^{eff}_{i-i',j-j'} \rho_{i',j'}$$

- For long beam in a conducting pipe, if grid length in z is >> pipe radius, can truncate at nearest neighbors:

$$\phi_{i,j} = \sum_{i'=1}^{N_x} (G^{eff}_{i-i',j-1} \rho_{i',j-1} + G^{eff}_{i-i',j} \rho_{i',j} + G^{eff}_{i-i',j+1} \rho_{i',j+1})$$

- For a rectangular pipe, can rewrite Green function as a sum of convolutions and correlations; then can still use FFT-based approach to sum over elements